

THE LIE - TROTTER INTEGRATOR IN THE DYNAMICS OF THE SYMMETRIC FREE RIGID BODY

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Abstract. The numerical integration plays a fundamental role in understanding the behaviour of many mechanical systems. In this paper some important aspects of the mechanical integrators on the dynamics of a mechanical system are studied. More specific, we have shown that if that the Lie-Trotter integrator is obtained, in case of Euler equations for the dynamics of symmetric free rigid body, then it is a Poisson integrator. At the end of the paper some important remarks are presented.

Keywords: Integrator; rigid body; symmetrical rigid body; mechanical system; dynamics.

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1. Introduction:

The overall situation for mechanical integrators is a complex one and it is still evolving. There are numerical integration methods that preserve some of the invariants of the mechanical system, such as: energy, momentum, or the symplectic form.

It is well known that if the energy and momentum map include all the integrals from a certain class that one cannot create integrators that are symplectic, energy preserving and momentum preserving unless they coincidentally integrate the equations exactly up to a time parametrization [6]. In mechanics the numerical integration plays a fundamental role.

Because there are many mechanical systems whose explicit integration is unknown, in our effort to understand their behavior, it is very useful the numerical integration of their dynamics.

Recently, more research is dedicated to the use of the mechanical integrators in molecular dynamics, spin systems, magnetism, etc.

2. Numerical and symplectic integrators

Definition 2.1. A numerical integrator on \mathbb{R}^n consists in a number of applications differentiable on class C^∞

$$\phi_t : \mathbb{R}^n \rightarrow \mathbb{R}^n,$$

which are differentiable in relation to $t \in \mathbb{R}$. We write

$$x_{n+1} = \phi_t(x_n).$$

We consider in \mathbb{R}^n the system of differential equations given by

$$\dot{x} = f(x), \quad (2.1)$$

where $x \in \mathbb{R}^n$ and $f \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$.

In the following, we will present a series of numerical integrators that enable us to approximate the solutions of the system (2.1).

(i) The Gauss-Legendre integrator, given by

$$\frac{x_{n+1} - x_n}{h} = f\left(\frac{x_{n+1} + x_n}{2}\right). \quad (2.2)$$

(ii) The Runge-Kutta integrator with s steps, given by

$$\begin{cases} \frac{x_{n+1} - x_n}{h} = \sum_{i=1}^s b_i f(X_i), \\ X_i = x_n + \sum_{j=1}^s a_{ij} f(X_j). \end{cases} \quad (2.3)$$

(iii) The Euler integrator, given by

$$\frac{x_{n+1} - x_n}{h} = f(x_n). \quad (2.4)$$

(iv) The modified Euler integrator, given by

$$\frac{x_{n+1} - x_n}{h} = f(x_n) + f(x_{n+1}). \quad (2.5)$$

(For other examples, see [3] and [9]).

Let (M, ω, H) be a mechanical Hamiltonian system.

Definition 2.2. A numerical integrator $\{\phi_t\}_{t \in \mathbb{R}}$ on M is called symplectic integrator if

$$\phi_t^* \omega = \omega, \quad (\forall) t \in \mathbb{R}.$$

Example 2.1. Considering a mechanical Hamiltonian system (M, ω, H) , where we have

$$M = T^*\mathbb{R} \simeq \mathbb{R}^2, \quad \omega = dp \wedge dq, \quad H(p, q) = \frac{1}{2}(q^2 + p^2).$$

Then the Ruth integrator associated with this dynamic

$$\begin{cases} \dot{q} = p, \\ \dot{p} = -q, \end{cases}$$

will be given as

$$\begin{cases} x_{n+1}^1 = x_n^1 + hx_n^2, \\ x_{n+1}^2 = -hx_n^1 + (1 - h^2) x_n^2. \end{cases} \quad (2.6)$$

The conclusions that can be drawn immediately, are

(i) The Integrator (2.6) doesn't conserve energy, because

$$H(x_{n+1}^1, x_{n+1}^2) = (1 + h^2) H(x_n^1, x_n^2) + h^2 \left(\frac{h^2}{2} - 1 \right) x_n^2 + h^3 x_n^1 x_n^2.$$

(ii) The integrator (2.6) is a symplectic integrator

More exactly we have

$$dx_{n+1}^2 \wedge dx_{n+1}^1 = dx_n^2 \wedge dx_n^1.$$

Proposition 2.1. ([5]) Let the Hamiltonian mechanical system

$$(\mathbb{R}^{2n}, \omega, H),$$

where

$$\omega = dp_1 \wedge dq^1 + \dots + dp_n \wedge dq^n.$$

Then the corresponding Gauss - Legendre integrator is a symplectic integrator.

Proposition 2.2. ([7], [15], [17]) Let the Hamiltonian mechanical system $(\mathbb{R}^{2n}, \omega, H)$, where

$$\omega = dp_1 \wedge dq^1 + \dots + dp_n \wedge dq^n.$$

Then the Runge - Kutta integrator with s stairs and h step is a symplectic integrator if and only if

$$\begin{cases} b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \\ 1 \leq i, j \leq s. \end{cases} \quad (2.7)$$

Definition 2.3. Let (M, ω, H, G) be a mechanical Hamiltonian system with symmetry having an application moment

$$J : M \rightarrow \mathcal{G}^*.$$

An integrator $\{\phi_t\}_{t \in \mathbb{R}}$ on M is called integrator moment if

$$\phi_t^* J = J, \quad (\forall) \quad t \in \mathbb{R}.$$

Proposition 2.3. ([6]) Let (M, ω, H, G) be a mechanical Hamiltonian system with symmetry and having a moment application

$$J : M \rightarrow \mathcal{G}^*.$$

Then any integrator $\{\phi_t\}_{t \in \mathbb{R}}$ on M which is G -invariant and is symplectic, is a moment integrator.

Proposition 2.4. ([6]) Let (M, ω, H, G) a mechanical Hamiltonian system with symmetry and having a moment application

$$J : M \rightarrow \mathcal{G}.$$

Then if $\{\phi_t\}_{t \in \mathbb{R}}$ is an integrator on M such that

- (i) $\{\phi_t\}_{t \in \mathbb{R}}$ is a symplectic integrator,
- (ii) $\{\phi_t\}_{t \in \mathbb{R}}$ is an energy integrator,
- (iii) $\{\phi_t\}_{t \in \mathbb{R}}$ is a moment integrator,
- (iv) dynamics on the reduced space (M_0, ω_0) not integrable.

Then $\{\phi_t\}_{t \in \mathbb{R}}$ gives the exact solution for initial system dynamics (unreduced).

Observation 2.1. Higher order integrators have generally similar properties. For details see [14], [10], [4], [19] and [16].

3. Poisson integrators

Let $(P, \{\cdot, \cdot\})$ be a dimensional finite Poisson manifold from class C^∞ .

Definition 3.1. An integrator $\{\phi_t\}_{t \in \mathbb{R}}$ on P is called Poisson integrator if

$$\phi_t^* \{f, g\} = \{\phi_t^* f, \phi_t^* g\}, \quad (\forall) f, g \in C^\infty(P, \mathbb{R}). \quad (3.1)$$

Observation 3.1. In the particular case $P = \mathbb{R}^n$, relation (8) is equivalent to

$$\begin{cases} (D\phi_t(x)) \cdot \Pi \cdot (D\phi_t(x))^t = \Pi(\phi_t(x)), \\ (\forall) t \in \mathbb{R}, (\forall) x \in \mathbb{R}^n, \end{cases} \quad (3.2)$$

where $D\phi_t$ designate Fréchet differential of ϕ_t , and Π is the matrix associated to the Poisson structure $\{\cdot, \cdot\}$, hence $\Pi = [\{x_i, x_j\}]$.

Example 3.1. ([11]) Let (\mathbb{R}^2, Π, H) be a Hamilton-Poisson mechanical system, where

$$\Pi = \begin{bmatrix} 0 & x_2 \\ -x_2 & 0 \end{bmatrix},$$

and

$$H(x_1, x_2) = Ax_1 + Bx_2 + C,$$

$A, B, C \in \mathbb{R}$. A simple calculation shows that

(i) The Runge - Kutta integrator with 1- step is a Poisson integrator if and only if

$$\begin{cases} h = \frac{1}{2bA - aA}, \\ 2bA - aA \neq 0. \end{cases}$$

(ii) The Runge - Kutta integrator with 1- step is an energy integrator if and only if

$$A = 0, \text{ sau } B = 0.$$

(iii) The Gauss-Legendre integrator is a Poisson integrator,

(iv) The Gauss-Legendre integrator is an energy integrator.

Proposition 3.1. ([8]) Let $(\mathbb{R}^n, \{\cdot, \cdot\}, H)$ be a Hamilton-Poisson mechanical system. If the matrix Π is constant, then the Runge-Kutta integrator with s -steps is a Poisson integrator if and only if

$$\begin{cases} b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \\ 1 \leq i, j \leq s. \end{cases}.$$

Observation 3.2. In the particular case $n = 2m$ and $\Pi = \begin{bmatrix} 0_m & I_m \\ -I_m & 0_m \end{bmatrix}$ the theorem [7], [15] and [17] is found (see **Proposition 2.2**).

Proposition 3.2. ([1]) Let $(\mathbb{R}^n, \{\cdot, \cdot\}, H)$ be a Hamilton-Poisson mechanical system. If the matrix Π is constant, then the Gauss-Legendre integrator is a Poisson integrator.

Observation 3.3. In the particular case $n = 2m$ and $\Pi = \begin{bmatrix} 0_m & I_m \\ -I_m & 0_m \end{bmatrix}$ the theorem [5] is found (see **Proposition 2.1**).

4. The Lie-Trotter Integrator and some properties in the dynamics of symmetric free rigid body

Let $(\mathbb{R}^n, \{\cdot, \cdot\}, H)$ be a Hamilton-Poisson mechanical system. The Lie-Trotter integrator (see [18]) usually applies when the Hamiltonian H can be written as

$$H = H_1 + H_2,$$

and the dynamics generated by X_{H_1} [resp X_{H_2}], hence $\exp(tX_{H_1})$ [resp. $\exp(tX_{H_2})$] can be explicitly integrated, hence $\exp(tX_{H_1})$ and $\exp(tX_{H_2})$ can be explicitly calculated. Then the Lie-Trotter integrator is given by

$$\phi_t(x) = [\exp(tX_{H_2}) \circ \exp(tX_{H_1})](x). \quad (4.1)$$

Because ϕ_t is actually composing two Hamiltonian flows, we have

Proposition 4.1. ([12], [13]) The Lie-Trotter integrator (4.1) has the following properties

(i) $\{\phi_t\}_{t \in \mathbb{R}}$ is a Poisson integrator,

(ii) The restriction of the foliation of a manifold symplectic Poisson $(\mathbb{R}^n, \{\cdot, \cdot\})$ gives rise to a symplectic integrator.

Obviously the integrator (4.1) is a first order integrator. This order can be grown by using some ideas from [2]. Concretely, a Poisson integrator of second order is given as

$$\phi_t^2(x) = \left[\exp\left(\frac{t}{2}X_{H_1}\right) \circ \exp(tX_{H_2}) \circ \exp\left(\frac{t}{2}X_{H_1}\right) \right](x).$$

The 4th order Poisson integrator is given by

$$\phi_t^4(x) = [\phi_t^2(x_1t) \circ \phi_t^2(x_0t) \circ \phi_t^2(x_1t)](x),$$

where

$$x_0 = \frac{\sqrt[3]{2}}{\sqrt[3]{2}-2}, \quad x_1 = \frac{1}{2-\sqrt[3]{2}}.$$

The process continues and, finally, it is obtained a Poisson integrator of the even order $2n+2$ defined as

$$\phi_t^{2n+2}(x) = [\phi_t^{2n}(x_1t) \circ \phi_t^{2n}(x_0t) \circ \phi_t^{2n}(x_1t)](x),$$

where

$$x_0 = \frac{\sqrt[2n+1]{2}}{\sqrt[2n+1]{2}-2}, \quad x_1 = \frac{1}{2-\sqrt[2n+1]{2}}.$$

Analogously explicit Poisson integrators can be build unconcerned their even order. We note that construction is difficult because in the construction of a Poisson integrator of even order $2n$, the second-order integrator ϕ_t^2 is used for 3^{n-1} times. Therefore the number of steps k is $1+3^{n-1}$, hence

$$k = 1 + 3^{n-1},$$

which grows extremely fast, and the calculations become increasingly more complex.

We proof below the next theorem:

Theorem 4.1. If the Lie - Trotter integrator is obtained, in the case of Euler equations for the dynamics of symmetric free rigid body, then it is a Poisson integrator.

Proof

The Euler equations for the dynamics of symmetric free rigid body are written as

$$\begin{cases} \dot{m}_1 = a_1 m_2 m_3, \\ \dot{m}_2 = -a_1 m_1 m_3, \\ \dot{m}_3 = 0, \end{cases} \quad (4.2)$$

where $a_1 = \frac{1}{I_3} - \frac{1}{I_1}$, the I_1, I_3 inertia tensors are components of the body and we assume in all that follows that $I_1 > I_3 > 0$.

As we well know (see some Puta's papers) the dynamic (4.2) has the following Hamilton-Poisson realization $((so(3))^* \simeq \mathbb{R}^3, \Pi, H)$, where

$$\Pi = \begin{bmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{bmatrix}, \quad H(m_1, m_2, m_3) = \frac{1}{2} \left(\frac{m_1^2}{I_1} + \frac{m_2^2}{I_1} + \frac{m_3^2}{I_3} \right).$$

We can say more and more precisely that the function $C \in C^\infty(\mathbb{R}^3, \mathbb{R})$ given by

$$C(m_1, m_2, m_3) = \frac{1}{2} (m_1^2 + m_2^2 + m_3^2),$$

is one Casimir of our configuration (\mathbb{R}^3, Π) . Actually, the symplectic foliation of the Poisson variety (\mathbb{R}^3, Π) is given by $\{0\}$ and by the coadjuncte orbits (O_k, ω_k) , where

$$O_k = \{(m_1, m_2, m_3) \in \mathbb{R}^3 \mid m_1^2 + m_2^2 + m_3^2 = k^2\},$$

and

$$\omega_k = \frac{1}{k} (m_2 dm_1 \wedge dm_3 - m_3 dm_1 \wedge dm_2 - m_1 dm_2 \wedge dm_3),$$

(ω_k is symplectic form Kirillov-Kostant-Souriau).

It can be now seen that the Hamiltonian field X_H splits

$$X_H = X_{H_1} + X_{H_2} + X_{H_3},$$

where

$$H_1(m_1, m_2, m_3) = \frac{1}{2I_1} m_1^2, \quad H_2(m_1, m_2, m_3) = \frac{1}{2I_1} m_2^2, \quad H_3(m_1, m_2, m_3) = \frac{1}{2I_3} m_3^2.$$

Then the corresponding flows have the following expressions

$$\begin{aligned} \begin{bmatrix} m_1(t) \\ m_2(t) \\ m_3(t) \end{bmatrix} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \frac{m_1(0)}{I_1} t & \sin \frac{m_1(0)}{I_1} t \\ 0 & -\sin \frac{m_1(0)}{I_1} t & \cos \frac{m_1(0)}{I_1} t \end{bmatrix} \begin{bmatrix} m_1(0) \\ m_2(0) \\ m_3(0) \end{bmatrix}, \\ \begin{bmatrix} m_1(t) \\ m_2(t) \\ m_3(t) \end{bmatrix} &= \begin{bmatrix} \cos \frac{m_2(0)}{I_1} t & 0 & -\sin \frac{m_2(0)}{I_1} t \\ 0 & 1 & 0 \\ \sin \frac{m_2(0)}{I_1} t & 0 & \cos \frac{m_2(0)}{I_1} t \end{bmatrix} \begin{bmatrix} m_1(0) \\ m_2(0) \\ m_3(0) \end{bmatrix}, \\ \begin{bmatrix} m_1(t) \\ m_2(t) \\ m_3(t) \end{bmatrix} &= \begin{bmatrix} \cos \frac{m_3(0)}{I_3} t & \sin \frac{m_3(0)}{I_3} t & 0 \\ -\sin \frac{m_3(0)}{I_3} t & \cos \frac{m_3(0)}{I_3} t & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} m_1(0) \\ m_2(0) \\ m_3(0) \end{bmatrix}. \end{aligned}$$

Then results that Lie - Trotter integrator has the following expression

$$\begin{bmatrix} m_1^{n+1} \\ m_2^{n+1} \\ m_3^{n+1} \end{bmatrix} = M \cdot N \cdot P \cdot \begin{bmatrix} m_1^n \\ m_2^n \\ m_3^n \end{bmatrix}, \quad (4.3)$$

where

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \frac{m_1(0)}{I_1} t & \sin \frac{m_1(0)}{I_1} t \\ 0 & -\sin \frac{m_1(0)}{I_1} t & \cos \frac{m_1(0)}{I_1} t \end{bmatrix},$$

$$N = \begin{bmatrix} \cos \frac{m_2(0)}{I_1} t & 0 & -\sin \frac{m_2(0)}{I_1} t \\ 0 & 1 & 0 \\ \sin \frac{m_2(0)}{I_1} t & 0 & \cos \frac{m_2(0)}{I_1} t \end{bmatrix},$$

$$P = \begin{bmatrix} \cos \frac{m_3(0)}{I_3} t & \sin \frac{m_3(0)}{I_3} t & 0 \\ -\sin \frac{m_3(0)}{I_3} t & \cos \frac{m_3(0)}{I_3} t & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

In conclusion the Lie-Trotter integrator (4.3) is a Poisson integrator.

From the above, (see [13]), we get

Proposition 4.2: The restriction of the coadjuncte orbits (O_k, ω_k) involves obtaining a symplectic integrator.

Proof: It results from the above theorem and **Proposition 4.1**.

Remark 4.1: The Lie-Trotter integrator is not an energy integrator.

Remark 4.2: If we compare with the Runge-Kutta integrator with 4 steps, then we obtain almost the same results, but the Lie - Trotter integrator has the advantage that it is much easier to implement.

Remark 4.3 Similar results with the ones presented in this paper are shown in [13] for the free rigid body. By analysing [13], one can see that some of the computations are identical.

Remark 4.4: It remains an open problem to find if there are characteristic roots of the matrix $M \cdot N \cdot P$ which have even values and follow a Hopf bifurcation moving from the unit circle on the real right so that their product is always 1 and if there is a transition in the dynamic integration (4.2) by means of the Lie - Trotter integrator, from the *real world* in the *complex world* tagged with the Hopf bifurcation for some of their values coming from $M \cdot N \cdot P$.

Remark 4.5 The square matrix $R = M \cdot N \cdot P$, where $\Pi_n = R^n \cdot \Pi_0$, $\Pi_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ can also give an open problem for finding if there are values of n so that the Markov chain related to the matrix can be found in a maximum possible number of states.

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